

On the Condition Number of the Total Least Squares Problem*

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Abstract

This paper concerns singular value decomposition (SVD)-based computable formulas and bounds for the condition number of the Total Least Squares (TLS) problem. For the TLS problem with the coefficient matrix A and the right-hand side b , a new closed formula is presented for the condition number. Unlike an important result in the literature that uses the SVDs of both A and $[A, b]$, our formula only requires the SVD of $[A, b]$. Based on the closed formula, both lower and upper bounds for the condition number are derived. It is proved that they are always sharp and estimate the condition number accurately. A few lower and upper bounds are further established that involve at most the smallest two singular values of A and of $[A, b]$. Tightness of these bounds is discussed, and numerical experiments are presented to confirm our theory and to demonstrate the improvement of our upper bounds over the upper bound due to Golub and Van Loan. Such lower and upper bounds are particularly useful for large scale TLS problems since they require the computation of only a few singular values of A and of $[A, b]$ other than all the singular values of them.

Keywords: total least squares, perturbation, condition number, singular value decomposition.

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1 Introduction

For given $A \in \mathbb{R}^{m \times n} (m > n)$, $b \in \mathbb{R}^m$, the TLS problem can be formulated as (see, e.g., [2, 6, 16])

$$\min \| [E, f] \|_F, \quad \text{subject to} \quad b + f \in \mathcal{R}(A + E), \quad (1)$$

where $\| \cdot \|_F$ denotes the Frobenius norm of a matrix and $\mathcal{R}(\cdot)$ denotes the range space. Suppose that $[E_{TLS}, f_{TLS}]$ solves the above problem. Then $x = x_{TLS}$ that satisfies the

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equation $(A + E_{TLS})x = b + f_{TLS}$ is called the TLS solution of (1). The TLS problem is a formulation of the linear approximation problem $Ax \approx b$. In this paper, we concentrate on the inconsistent linear approximation problem, i.e., $b \notin \mathcal{R}(A)$. Otherwise, $[E_{TLS}, f_{TLS}] = O$, the zero matrix.

Given a problem, the condition number measures the worst-case sensitivity of its solution to small perturbations in the input data. It is well known that the condition number is independent of perturbations themselves and is expressed by some information on the original data. Combined with backward errors, it provides a (possibly approximate) linear upper bound for the forward error, i.e., the difference between a perturbed solution and the exact solution. Since the 1980's, algebraic perturbation analysis for the TLS problem has been made extensively; see [4, 6, 14, 20] and the references therein. From the expressions of perturbation bounds presented in [4, 6, 14, 20], we can see that there are some essential distinctions between them and a standard form. The perturbation bound in [6] is a standard one in the sense that it is expressed as some perturbation free factor times backward errors. So, this factor is naturally an upper bound for the TLS condition number. The perturbation bound in [20] is nonstandard and unusual since the perturbation bound is not zero when a perturbation is exactly zero. Actually, a careful observation reveals that the bound is never less than a certain positive constant under the assumption $b \notin \mathcal{R}(A)$. As a result, it makes no sense to extract an upper bound for the TLS condition number from this perturbation bound. The perturbations bounds in [4, 14] are very different from a standard perturbation bound in that they contain some information on the perturbed TLS problem, e.g., the TLS solution \tilde{x}_{TLS} of the perturbed TLS problem in [4] and the right singular vectors associated with the smallest singular values of both $[A, b]$ and its perturbed matrix in [14]. Because of these features and the fact that the condition number itself has nothing to do with perturbations, it is impossible to extract upper bounds for the TLS condition number from the perturbation bounds in [4, 14]. If one attempts to find suitable upper bounds for the TLS condition number, some further and complicated treatments are required and it is necessary to make each of their perturbation bounds become a standard one, that is, some perturbation free factor times the backward error.

In recent years, asymptotic perturbation analysis and TLS condition numbers have been investigated. The authors [13] and Zhou et al. [21] have presented a first order perturbation analysis of the TLS problem and established Kronecker products-based condition number formulas. Baboulin and Gratton [1] have derived a SVD-based closed formula for the TLS condition number and an upper bound for it that involve all the singular values and the right singular vectors of both A and $[A, b]$ and several singular values of them, respectively. To our best knowledge, however, there has been *no* lower bound available for the TLS condition number in the literature.

It is well known that the TLS solution x_{TLS} involves the smallest singular value and the corresponding right singular vector of $[A, b]$, see, e.g., [6]. Based on this intimate relation and motivated by the work of [1], we continue our work in [13] to study SVD-based TLS condition number theory. We will derive a number of results. Firstly, we establish a new closed formula of the TLS condition number. It is distinctive that, unlike the result in [1] that requires the SVDs of both A and $[A, b]$, our formula only uses the singular values and the right singular vectors of $[A, b]$. Secondly, starting with the closed formula, we present both *lower* and *upper* bounds for the condition number that involve the singular values of $[A, b]$ and the last entries of the right singular vectors of $[A, b]$. Furthermore, we prove that these bounds are always sharp and can estimate the condition number accurately. We then

focus on cheaply computable bounds for the TLS condition number. We establish *lower* and *upper* bounds that involve *at most the smallest two singular values* of A and of $[A, b]$. We discuss how tight the bounds are. These bounds are particularly useful for large scale TLS problems since they require to compute only a very few smallest singular values of A and $[A, b]$ other than all the singular values of them. So we can compute these bounds by using some iterative solvers for large SVDs, e.g., [10, 11]. From [6], as mentioned previously, an upper bound for the TLS condition number can be extracted. It has been simplified and applied to evaluate the conditioning of the TLS problem in [3]. We will present numerical experiments to demonstrate great improvements of our upper bounds over the upper bound due to Golub and Van Loan [6].

The paper is organized as follows. In Section 2, we present some preliminaries necessary. In Section 3, we establish some useful and necessary results related to a specific orthogonal matrix. In Section 4, we present a new closed formula of the TLS condition number. The straightforward bounds for the TLS condition number are derived in Section 5. In Section 6, we report numerical experiments to show the tightness of our bounds for the TLS condition number and considerable improvements over Golub-Van Loan's bound. We conclude the paper with some remarks and future work in Section 7.

Throughout the paper, for given positive integers m, n , denote by \mathbb{R}^n the space of n -dimensional real column vectors, by $\mathbb{R}^{m \times n}$ the space of all $m \times n$ real matrices, and by $\|\cdot\|$ and $\|\cdot\|_F$ 2-norm and Frobenius norm of their arguments, respectively. Given a matrix A , $A(1:i, 1:j)$ is a Matlab notation that denotes the submatrix in the intersection of rows $1, \dots, i$ and columns $1, \dots, j$, and $\sigma_i(A)$ denotes the i th largest singular value of A . For a vector a , $a(i)$ denotes the i th component of a , and $\text{diag}(a)$ is a diagonal matrix whose diagonals are $a(i)$'s. I_n denotes the $n \times n$ identity matrix and $O_{m,n}$ denotes the $m \times n$ zero matrix with O a zero matrix whose dimension is clear from the context. For the matrices $A = [a_1, \dots, a_n] = [a_{ij}] \in \mathbb{R}^{m \times n}$ and B , $A \otimes B = [a_{ij}B]$ is the Kronecker product of A and B , and the linear operator $\text{vec} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}^{mn}$ is defined by $\text{vec}(A) = [a_1^T, \dots, a_n^T]^T$.

2 Preliminaries

Throughout the paper, let $A = \hat{U} \text{diag}(\hat{\sigma}_1, \dots, \hat{\sigma}_n) \hat{V}^T$ be the thin SVD of $A \in \mathbb{R}^{m \times n}$, where $\hat{\sigma}_1 \geq \dots \geq \hat{\sigma}_n$, $\hat{U} \in \mathbb{R}^{m \times n}$, $\hat{V} \in \mathbb{R}^{n \times n}$ and $\hat{U}^T \hat{U} = I_n$, $\hat{V}^T \hat{V} = I_n$, and let $[A, b] = U \text{diag}(\sigma_1, \dots, \sigma_{n+1}) V^T$ be the thin SVD of $[A, b] \in \mathbb{R}^{m \times (n+1)}$, where $\sigma_1 \geq \dots \geq \sigma_{n+1}$, $U = [u_1, \dots, u_{n+1}] \in \mathbb{R}^{m \times (n+1)}$, $V = [v_1, \dots, v_{n+1}] \in \mathbb{R}^{(n+1) \times (n+1)}$ and $U^T U = I_{n+1}$, $V^T V = I_{n+1}$.

The TLS problem (1) may not have a solution, but it does have a unique solution if the following condition holds [16]:

$$A \text{ has rank } n \text{ and } b \notin \mathcal{U}_{\min}, \quad (2)$$

where \mathcal{U}_{\min} denotes the left singular vector subspace of A corresponding to its smallest singular value. Throughout the paper, we always assume that (2) holds.

It is noted in [16] that condition (2) means $\sigma_{n+1} < \hat{\sigma}_n$, the existence and uniqueness condition of the TLS solution given in [6]. Under the condition that $\sigma_{n+1} < \hat{\sigma}_n$, it is proved

in [6] that

$$x_{TLS} = (A^T A - \sigma_{n+1}^2 I)^{-1} A^T b \quad (3)$$

$$= - \left[\frac{v_{n+1}(1)}{v_{n+1}(n+1)}, \dots, \frac{v_{n+1}(n)}{v_{n+1}(n+1)} \right]^T. \quad (4)$$

We comment that (2) implies that $A^T b \neq 0$. So $x_{TLS} \neq 0$.

Given the TLS problem (1), let $\tilde{A} = A + \Delta A$, $\tilde{b} = b + \Delta b$, where ΔA and Δb denote the perturbations in A and b , respectively. Consider the perturbed TLS problem

$$\min \| [E, f] \|_F \text{ subject to } \tilde{b} + f \in \mathcal{R}(\tilde{A} + E). \quad (5)$$

Under the assumption that $b \notin \mathcal{R}(A)$, it follows from (2) that $0 < \sigma_{n+1} < \hat{\sigma}_n$. In [13], the following result is established for the TLS solution \tilde{x}_{TLS} of the perturbed TLS problem (5).

Theorem 1 *Suppose that the TLS problem (1) satisfies $0 < \sigma_{n+1} < \hat{\sigma}_n$. Define $r = Ax_{TLS} - b$ and $G = [x_{TLS}^T, -1] \otimes I_m \in \mathbb{R}^{m \times (mn+m)}$. If $\| [\Delta A, \Delta b] \|_F$ is small enough, then the perturbed problem (5) has a unique TLS solution \tilde{x}_{TLS} . Moreover,*

$$\tilde{x}_{TLS} = x_{TLS} + K \begin{bmatrix} \text{vec}(\Delta A) \\ \Delta b \end{bmatrix} + \mathcal{O}(\| [\Delta A, \Delta b] \|_F^2), \quad (6)$$

where

$$K = (A^T A - \sigma_{n+1}^2 I_n)^{-1} \left(2A^T \frac{r}{\|r\|} \frac{r^T}{\|r\|} G - A^T G - [I_n \otimes r^T, O_{n,m}] \right) \in \mathbb{R}^{n \times (mn+m)}. \quad (7)$$

It is shown in [6] that

$$\sigma_{n+1}^2 = \frac{\|r\|^2}{1 + \|x_{TLS}\|^2} \quad (8)$$

and

$$A^T r = \frac{\|r\|^2}{1 + \|x_{TLS}\|^2} x_{TLS} = \sigma_{n+1}^2 x_{TLS}. \quad (9)$$

From (4), it follows that

$$v_{n+1} = \frac{1}{\sqrt{1 + \|x_{TLS}\|^2}} \begin{bmatrix} x_{TLS} \\ -1 \end{bmatrix} \quad (10)$$

up to a sign ± 1 . We will use the above two relations later. The following basic properties of the Kronecker products of matrices can be found in [8] and are needed later:

$$\begin{aligned} (A_1 \otimes A_3)(A_2 \otimes A_4) &= (A_1 A_2) \otimes (A_3 A_4), \\ (A_1 \otimes A_2)^T &= A_1^T \otimes A_2^T, \end{aligned}$$

where $A_i, i = 1, \dots, 4$ are matrices with appropriate sizes.

3 Some results related to a specific orthogonal matrix

In this section, we establish a number of results that are related to a specific orthogonal matrix. They play a central role in deriving our lower and upper bounds for the condition number of the TLS problem in the next section.

Proposition 1 *Let W be an arbitrary $(n+1) \times (n+1)$ orthogonal matrix with $W(n+1, n+1) = -\alpha$, $0 < \alpha < 1$. Denote $W_{11} = W(1:n, 1:n)$. Then*

$$\sigma_1(W_{11}) = \cdots = \sigma_{n-1}(W_{11}) = 1, \quad \sigma_n(W_{11}) = \alpha. \quad (11)$$

Furthermore, W can be written as

$$W = \begin{bmatrix} W_{11} & \sqrt{1-\alpha^2} \bar{u}_n \\ \sqrt{1-\alpha^2} \bar{v}_n^T & -\alpha \end{bmatrix}, \quad (12)$$

where \bar{u}_n and \bar{v}_n are the left and right singular vectors associated with the smallest singular value of W_{11} .

Proof. It is an immediate result of Theorem 2.6.3 in [7]. \square

Let $[\bar{\beta}_1, \dots, \bar{\beta}_n, -\alpha]$ be the last row of W . From (12) we have

$$\bar{v}_n^T = \frac{1}{\sqrt{1-\alpha^2}} [\bar{\beta}_1, \dots, \bar{\beta}_n]. \quad (13)$$

Since $(\alpha^{-1}, \bar{u}_n, \bar{v}_n)$ is the largest singular triplet of W_{11}^{-T} , from (11) we get the SVD of W_{11}^{-T} :

$$W_{11}^{-T} = \alpha^{-1} \bar{u}_n \bar{v}_n^T + \sum_{i=1}^{n-1} \bar{u}_i \bar{v}_i^T,$$

where $\bar{u}_i, \bar{v}_i, i = 1, \dots, n-1$ represent the left and right singular vectors associated with the singular value one. Then, by (13) we obtain

$$W_{11}^{-T} = [\alpha^{-1} \bar{u}_n, \bar{u}_1, \dots, \bar{u}_{n-1}] \begin{bmatrix} \frac{\bar{\beta}_1}{\sqrt{1-\alpha^2}} & \cdots & \frac{\bar{\beta}_n}{\sqrt{1-\alpha^2}} \\ \bar{v}_1(1) & \cdots & \bar{v}_1(n) \\ \vdots & \cdots & \vdots \\ \bar{v}_{n-1}(1) & \cdots & \bar{v}_{n-1}(n) \end{bmatrix} \quad (14)$$

$$= \left[\frac{\alpha^{-1} \bar{\beta}_1}{\sqrt{1-\alpha^2}} \bar{u}_n + w_1, \dots, \frac{\alpha^{-1} \bar{\beta}_n}{\sqrt{1-\alpha^2}} \bar{u}_n + w_n \right], \quad (15)$$

where $\bar{v}_i(k)$ denotes the k th component of \bar{v}_i and

$$w_k = \sum_{i=1}^{n-1} \bar{v}_i(k) \bar{u}_i, \quad k = 1, \dots, n. \quad (16)$$

From (14) we get

$$\sqrt{\sum_{i=1}^{n-1} \bar{v}_i^2(n)} = \frac{\sqrt{1-\alpha^2-\bar{\beta}_n^2}}{\sqrt{1-\alpha^2}}, \quad (17)$$

which will be used later.

Before proceeding, we need the following lemma.

Lemma 1 For given matrices $A_1, A_2 \in \mathbb{R}^{n \times n}$, if $A_1^T A_2 = O$, then

$$\frac{1}{2}(\|A_1\| + \|A_2\|) \leq \|A_1 + A_2\| \leq \|A_1\| + \|A_2\|. \quad (18)$$

Proof. The upper bound in (18) is obvious. It suffices to prove the lower one. For an arbitrary vector $x \in \mathbb{R}^n$, from $(A_1 x)^T (A_2 x) = 0$ it follows that

$$\|A_1 x\|, \|A_2 x\| \leq \|A_1 x + A_2 x\|$$

and that

$$\begin{aligned} \|A_1\| &= \max_{\|x\|=1} \|A_1 x\| \leq \max_{\|x\|=1} \|A_1 x + A_2 x\| = \|A_1 + A_2\|, \\ \|A_2\| &= \max_{\|x\|=1} \|A_2 x\| \leq \max_{\|x\|=1} \|A_1 x + A_2 x\| = \|A_1 + A_2\|. \end{aligned}$$

So, the assertion is proved. \square

Now we are in a position to show the following two propositions.

Proposition 2 Let W be an arbitrary $(n+1) \times (n+1)$ orthogonal matrix with $W(n+1, n+1) = -\alpha$, $0 < \alpha < 1$. Let $W_{11} = W(1:n, 1:n)$ and $[\bar{\beta}_1, \dots, \bar{\beta}_n, -\alpha]$ be the last row of W . Then for $\bar{S} = \text{diag}([\bar{s}_1, \dots, \bar{s}_n])$ with $\bar{s}_1, \dots, \bar{s}_n$ arbitrary positive numbers ordered as $0 < \bar{s}_1 \leq \bar{s}_2 \leq \dots \leq \bar{s}_n$, we have

$$\begin{aligned} \underline{c} &:= \frac{1}{2} \left(\frac{\alpha^{-1} \sqrt{\bar{\beta}_1^2 \bar{s}_1^2 + \dots + \bar{\beta}_n^2 \bar{s}_n^2}}{\sqrt{1-\alpha^2}} + \frac{\sqrt{1-\alpha^2-\bar{\beta}_n^2}}{\sqrt{1-\alpha^2}} \bar{s}_n \right) \\ &\leq \|W_{11}^{-T} \bar{S}\| \leq \bar{c} := \frac{\alpha^{-1} \sqrt{\bar{\beta}_1^2 \bar{s}_1^2 + \dots + \bar{\beta}_n^2 \bar{s}_n^2}}{\sqrt{1-\alpha^2}} + \bar{s}_n. \end{aligned} \quad (19)$$

Proof. Following (15), we get

$$W_{11}^{-T} \bar{S} = \left[\frac{\alpha^{-1} \bar{\beta}_1 \bar{s}_1}{\sqrt{1-\alpha^2}} \bar{u}_n + \bar{s}_1 w_1, \dots, \frac{\alpha^{-1} \bar{\beta}_n \bar{s}_n}{\sqrt{1-\alpha^2}} \bar{u}_n + \bar{s}_n w_n \right].$$

Define the matrices

$$A_1 = \left[\frac{\alpha^{-1} \bar{\beta}_1 \bar{s}_1}{\sqrt{1-\alpha^2}} \bar{u}_n, \dots, \frac{\alpha^{-1} \bar{\beta}_n \bar{s}_n}{\sqrt{1-\alpha^2}} \bar{u}_n \right]$$

and

$$A_2 = W_{11}^{-T} \bar{S} - A_1 = [\bar{s}_1 w_1, \dots, \bar{s}_n w_n]. \quad (20)$$

Then

$$\|A_1\| = \frac{\alpha^{-1}}{\sqrt{1-\alpha^2}} \sqrt{\bar{\beta}_1^2 \bar{s}_1^2 + \dots + \bar{\beta}_n^2 \bar{s}_n^2}. \quad (21)$$

From (16) and (17) we obtain

$$\|w_n\| = \sqrt{\sum_{i=1}^{n-1} \bar{v}_i^2(n)} = \frac{\sqrt{1-\alpha^2-\bar{\beta}_n^2}}{\sqrt{1-\alpha^2}} \quad \text{and} \quad \|[w_1, \dots, w_n]\| = \left\| \sum_{i=1}^{n-1} \bar{u}_i \bar{v}_i^T \right\| = 1.$$

Furthermore, since $\|\bar{S}\| = \bar{s}_n$, it follows from

$$\|\bar{s}_n w_n\| \leq \|A_2\| \leq \|[w_1, \dots, w_n]\| \|\bar{S}\|$$

that

$$\frac{\sqrt{1 - \alpha^2 - \bar{\beta}_n^2}}{\sqrt{1 - \alpha^2}} \bar{s}_n \leq \|A_2\| \leq \bar{s}_n. \quad (22)$$

Note that $A_1^T A_2 = O$. Based on Lemma 1 and combining (20), (21) with (22), we establish the desired inequality. \square

Proposition 3 Suppose that $0 < \alpha \leq \frac{1}{2}$, where α is defined as in Proposition 2. Then for \underline{c} and \bar{c} in Proposition 2, we have

$$\underline{c} < \bar{c} < 4\underline{c}. \quad (23)$$

Proof. If $\frac{|\bar{\beta}_n|}{\sqrt{1 - \alpha^2}} < \frac{\sqrt{3}}{2}$, it is easy to verify that

$$\frac{\sqrt{1 - \alpha^2 - \bar{\beta}_n^2}}{\sqrt{1 - \alpha^2}} > \frac{1}{2}$$

and that

$$\underline{c} > \frac{1}{4}\bar{c}.$$

Thus, (23) holds. If $\frac{|\bar{\beta}_n|}{\sqrt{1 - \alpha^2}} \geq \frac{\sqrt{3}}{2}$, then

$$\alpha^{-1} \frac{|\bar{\beta}_n|}{\sqrt{1 - \alpha^2}} \geq \frac{\sqrt{3}}{2} \alpha^{-1} > 1,$$

so $\alpha^{-1} \frac{|\bar{\beta}_n|}{\sqrt{1 - \alpha^2}} \bar{s}_n > \bar{s}_n$, from which and the definitions of \bar{c} and \underline{c} it follows that

$$\begin{aligned} \bar{c} &< \frac{\alpha^{-1} \sqrt{\bar{\beta}_1^2 \bar{s}_1^2 + \dots + \bar{\beta}_n^2 \bar{s}_n^2}}{\sqrt{1 - \alpha^2}} + \alpha^{-1} \frac{|\bar{\beta}_n|}{\sqrt{1 - \alpha^2}} \bar{s}_n \\ &\leq \frac{2\alpha^{-1} \sqrt{\bar{\beta}_1^2 \bar{s}_1^2 + \dots + \bar{\beta}_n^2 \bar{s}_n^2}}{\sqrt{1 - \alpha^2}} \\ &\leq \frac{2\alpha^{-1} \sqrt{\bar{\beta}_1^2 \bar{s}_1^2 + \dots + \bar{\beta}_n^2 \bar{s}_n^2}}{\sqrt{1 - \alpha^2}} + \frac{2\sqrt{1 - \alpha^2 - \bar{\beta}_n^2}}{\sqrt{1 - \alpha^2}} \bar{s}_n = 4\underline{c}. \end{aligned}$$

Thus, (23) still holds. \square

This proposition means that the upper bound is at most four times of the lower bound in Proposition 2. So we can estimate $\|W_{11}^{-T} \bar{S}\|$ accurately by its lower or upper bound within no more than four times of the exact $\|W_{11}^{-T} \bar{S}\|$.

4 A closed formula for the TLS condition number

Throughout the paper, we follow the definition of condition number in [5, 18]. Let $g : \mathbb{R}^p \rightarrow \mathbb{R}^q$ be a continuous map in normed linear spaces defined on an open set $D_g \subset \mathbb{R}^p$. For a given $a_0 \in D_g$, $a_0 \neq 0$, with $g(a_0) \neq 0$, if g is differentiable at a_0 , then the absolute condition number of g at a_0 is

$$\kappa_g(a_0) = \|g'(a_0)\|, \quad (24)$$

and the relative condition number is

$$\kappa_g^{\text{rel}}(a_0) = \frac{\|g'(a_0)\| \|a_0\|}{\|g(a_0)\|}, \quad (25)$$

where $g'(a_0) \in \mathbb{R}^{q \times p}$ denotes the derivative of g at a_0 .

In [1], a SVD-based closed formula for the condition number of the TLS problem was presented. Denote by $\kappa_g(A, b)$ the absolute TLS condition number. It was shown in [1] that

$$\kappa_g(A, b) = \sqrt{\|x_{TLS}\|^2 + 1} \left\| \hat{D} [\hat{V}^T, O_{n,1}] V [D, O_{n,1}]^T \right\|, \quad (26)$$

where

$$\begin{aligned} \hat{D} &= \text{diag} \left(\left[\frac{1}{\hat{\sigma}_1^2 - \sigma_{n+1}^2}, \dots, \frac{1}{\hat{\sigma}_n^2 - \sigma_{n+1}^2} \right] \right), \\ D &= \text{diag} \left(\left[\sqrt{\sigma_1^2 + \sigma_{n+1}^2}, \dots, \sqrt{\sigma_n^2 + \sigma_{n+1}^2} \right] \right). \end{aligned}$$

Next we will derive a new SVD-based formula for the TLS condition number. It is distinctive that, unlike (26) that involves the singular values and right singular vectors of both $[A, b]$ and A , our formula only uses those of $[A, b]$.

Denote $a = \text{vec}(A)$ and define the following function in a small neighborhood of $[a^T, b^T]^T \in \mathbb{R}^{m(n+1)}$:

$$\begin{aligned} g : \mathbb{R}^{m(n+1)} &\longrightarrow \mathbb{R}^n \\ \begin{bmatrix} \tilde{a} \\ \tilde{b} \end{bmatrix} &\longmapsto \tilde{x}_{TLS} = (\tilde{A}^T \tilde{A} - \tilde{\sigma}_{n+1}^2 I_n)^{-1} \tilde{A}^T \tilde{b}, \end{aligned}$$

where $\tilde{a} = a + \text{vec}(\Delta A) = \text{vec}(\tilde{A})$, $\tilde{b} = b + \Delta b$. Then we have $g([a^T, b^T]^T) = x_{TLS}$. Based on Theorem 1, we can present the following result.

Theorem 2 *Given the TLS problem (1), let $\kappa_g(A, b)$ and $\kappa_g^{\text{rel}}(A, b)$ be the absolute and relative condition numbers of the TLS problem, respectively. Then*

$$\kappa_g(A, b) = \|K\|, \quad \kappa_g^{\text{rel}}(A, b) = \frac{\|K\| \| [A, b] \|_F}{\|x_{TLS}\|}, \quad (27)$$

where K is defined as in (7).

Proof. Recall that our TLS problem satisfies $0 < \sigma_{n+1} < \hat{\sigma}_n$. By Theorem 1 and the definition of g , we see that g is differentiable at $[a^T, b^T]^T$ and $g'([a^T, b^T]^T) = K$. Then the assertion follows from (24) and (25). \square

Now we can establish our computable formula for the TLS condition number.

Theorem 3 Given the TLS problem (1), let $[A, b] = U \text{diag}(\sigma_1, \dots, \sigma_{n+1}) V^T$ be the thin SVD of $[A, b]$ with $V_{11} = V(1:n, 1:n)$. Then

$$\kappa_g(A, b) = \sqrt{\|x_{TLS}\|^2 + 1} \|V_{11}^{-T} S\|, \quad (28)$$

where $S = \text{diag}([s_1, \dots, s_n])$ with $s_i = \frac{\sqrt{\sigma_i^2 + \sigma_{n+1}^2}}{\sigma_i^2 - \sigma_{n+1}^2}$, $i = 1, \dots, n$.

Proof. Consider expression (7) of K . By the properties of Kronecker product of matrices, we get

$$GG^T = ([x_{TLS}^T, -1] \otimes I_m) \left(\begin{bmatrix} x_{TLS} \\ -1 \end{bmatrix} \otimes I_m \right) = (\|x_{TLS}\|^2 + 1) I_m,$$

$$[I_n \otimes r^T, O_{n,m}] G^T = [I_n \otimes r^T, O_{n,m}] \begin{bmatrix} x_{TLS} \otimes I_m \\ -I_m \end{bmatrix} = (I_n \otimes r^T)(x_{TLS} \otimes I_m) = x_{TLS} r^T$$

and

$$[I_n \otimes r^T, O_{n,m}] \begin{bmatrix} I_n \otimes r \\ O_{m,n} \end{bmatrix} = (I_n \otimes r^T)(I_n \otimes r) = \|r\|^2 I_n.$$

Thus, we have

$$\begin{aligned} & \left(2A^T \frac{r}{\|r\|} \frac{r^T}{\|r\|} G - A^T G - [I_n \otimes r^T, O_{n,m}] \right) \\ & \cdot \left(2G^T \frac{r}{\|r\|} \frac{r^T}{\|r\|} A - G^T A - \begin{bmatrix} I_n \otimes r \\ O_{m,n} \end{bmatrix} \right) \\ & = (\|x_{TLS}\|^2 + 1) A^T A + \|r\|^2 I_n - x_{TLS} r^T A - A^T r x_{TLS}^T \\ & = (\|x_{TLS}\|^2 + 1) A^T A + \|r\|^2 I_n - 2\sigma_{n+1}^2 x_{TLS} x_{TLS}^T, \end{aligned}$$

during which the last equality made use of the relation $A^T r x_{TLS}^T = \sigma_{n+1}^2 x_{TLS} x_{TLS}^T$ that is obtained from (9). Denote $P = A^T A - \sigma_{n+1}^2 I_n$. We get

$$\begin{aligned} KK^T &= P^{-1} ((\|x_{TLS}\|^2 + 1) A^T A + \|r\|^2 I_n - 2\sigma_{n+1}^2 x_{TLS} x_{TLS}^T) P^{-1} \\ &= (\|x_{TLS}\|^2 + 1) P^{-1} \left(A^T A + \sigma_{n+1}^2 I_n - \frac{2\sigma_{n+1}^2 x_{TLS} x_{TLS}^T}{\|x_{TLS}\|^2 + 1} \right) P^{-1} \quad (29) \end{aligned}$$

$$= (\|x_{TLS}\|^2 + 1) \left(P^{-1} + 2\sigma_{n+1}^2 P^{-1} \left(I_n - \frac{x_{TLS} x_{TLS}^T}{1 + \|x_{TLS}\|^2} \right) P^{-1} \right), \quad (30)$$

during which the second equality used (8). Denote $V = [v_1, \dots, v_{n+1}]$ and note that

$$\begin{aligned} [A, b]^T [A, b] - \sigma_{n+1}^2 I_{n+1} &= \sum_{i=1}^{n+1} \sigma_i^2 v_i v_i^T - \sigma_{n+1}^2 \sum_{i=1}^{n+1} v_i v_i^T \\ &= \sum_{i=1}^n (\sigma_i^2 - \sigma_{n+1}^2) v_i v_i^T. \end{aligned}$$

We get

$$\begin{aligned}
P &= [I_n, O] \sum_{i=1}^n (\sigma_i^2 - \sigma_{n+1}^2) v_i v_i^T \begin{bmatrix} I_n \\ O \end{bmatrix} \\
&= [I_n, O] [v_1, \dots, v_n] \begin{bmatrix} \sigma_1^2 - \sigma_{n+1}^2 & & \\ & \ddots & \\ & & \sigma_n^2 - \sigma_{n+1}^2 \end{bmatrix} \begin{bmatrix} v_1^T \\ \vdots \\ v_n^T \end{bmatrix} \begin{bmatrix} I_n \\ O \end{bmatrix} \\
&= V_{11} \text{diag}(\sigma_1^2 - \sigma_{n+1}^2, \dots, \sigma_n^2 - \sigma_{n+1}^2) V_{11}^T := V_{11} \Lambda V_{11}^T.
\end{aligned} \tag{31}$$

Similarly, since $v_{n+1} = \frac{1}{\sqrt{1+\|x_{TLS}\|^2}} \begin{bmatrix} x_{TLS} \\ -1 \end{bmatrix}$ (c.f. (10)), we have

$$I_{n+1} - \frac{1}{1 + \|x_{TLS}\|^2} \begin{bmatrix} x_{TLS} x_{TLS}^T & -x_{TLS} \\ -x_{TLS} & 1 \end{bmatrix} = I_{n+1} - v_{n+1} v_{n+1}^T = [v_1, \dots, v_n] \begin{bmatrix} v_1^T \\ \vdots \\ v_n^T \end{bmatrix}$$

and

$$I_n - \frac{x_{TLS} x_{TLS}^T}{1 + \|x_{TLS}\|^2} = V_{11} V_{11}^T. \tag{32}$$

Combining (31) and (32), we have

$$\begin{aligned}
&P^{-1} + 2\sigma_{n+1}^2 P^{-1} \left(I_n - \frac{x_{TLS} x_{TLS}^T}{1 + \|x_{TLS}\|^2} \right) P^{-1} \\
&= V_{11}^{-T} \Lambda^{-1} V_{11}^{-1} + 2\sigma_{n+1}^2 \left(V_{11}^{-T} \Lambda^{-1} V_{11}^{-1} \right) V_{11} V_{11}^T \left(V_{11}^{-T} \Lambda^{-1} V_{11}^{-1} \right) \\
&= V_{11}^{-T} \Lambda^{-1} V_{11}^{-1} + 2\sigma_{n+1}^2 V_{11}^{-T} \Lambda^{-2} V_{11}^{-1} \\
&= V_{11}^{-T} (\Lambda^{-1} + 2\sigma_{n+1}^2 \Lambda^{-2}) V_{11}^{-1} = \left(V_{11}^{-T} S \right) \left(V_{11}^{-T} S \right)^T.
\end{aligned} \tag{33}$$

Then it follows from (30) and Theorem 2 that the desired equality holds. \square

By Theorem 3, we can calculate $\kappa_g(A, b)$ by inverting V_{11}^T . Next we show that the condition number of V_{11}^T is exactly $\sqrt{1 + \|x_{TLS}\|^2}$.

Theorem 4 *Under the conditions of Theorem 3, we have*

$$\sigma_1(V_{11}) = \dots = \sigma_{n-1}(V_{11}) = 1, \sigma_n(V_{11}) = \frac{1}{\sqrt{1 + \|x_{TLS}\|^2}} \tag{34}$$

and

$$\kappa(V_{11}) = \frac{\sigma_1(V_{11})}{\sigma_n(V_{11})} = \sqrt{1 + \|x_{TLS}\|^2}. \tag{35}$$

Proof. By (10) we get $V(n+1, n+1) = -\frac{1}{\sqrt{1+\|x_{TLS}\|^2}}$. Recalling that $x_{TLS} \neq 0$, we get $\frac{1}{\sqrt{1+\|x_{TLS}\|^2}} < 1$. Applying Proposition 1, we prove the theorem. \square

5 Straightforward bounds for the TLS condition number

5.1 Sharp lower and upper bounds based on the SVD of $[A, b]$

In this subsection, we further investigate our result in Theorem 3 and show how to estimate $\kappa_g(A, b)$ accurately without computing $\|V_{11}^{-T}S\|$, i.e., avoiding inverting V_{11}^T .

For the TLS problem (1), from now on we denote $\alpha = -V(n+1, n+1)$. By (10) we get

$$\alpha = \frac{1}{\sqrt{1 + \|x_{TLS}\|^2}}. \quad (36)$$

Recalling that $x_{TLS} \neq 0$, we have $0 < \alpha < 1$. Then we have the following theorem.

Theorem 5 *For the TLS problem (1), it holds that*

$$\underline{\kappa} := \alpha^{-1} \frac{\sqrt{\sigma_n^2 + \sigma_{n+1}^2}}{\sigma_n^2 - \sigma_{n+1}^2} \leq \kappa_g(A, b) \leq \bar{\kappa} := \alpha^{-2} \frac{\sqrt{\sigma_n^2 + \sigma_{n+1}^2}}{\sigma_n^2 - \sigma_{n+1}^2}. \quad (37)$$

Proof. As before, let $[A, b] = U \text{diag}(\sigma_1, \dots, \sigma_{n+1}) V^T$ be its thin SVD with $V_{11} = V(1 : n, 1 : n)$. From (34) it follows that

$$\sigma_n(V_{11}^{-T}) = (\sigma_1(V_{11}))^{-1} = 1, \quad \sigma_1(V_{11}^{-T}) = (\sigma_n(V_{11}))^{-1} = \alpha^{-1}. \quad (38)$$

Define $S = \text{diag}([s_1, \dots, s_n])$ with $s_i = \frac{\sqrt{\sigma_i^2 + \sigma_{n+1}^2}}{\sigma_i^2 - \sigma_{n+1}^2}$, $i = 1, \dots, n$. We then have

$$s_n = \sigma_n(V_{11}^{-T}) \|S\| \leq \|V_{11}^{-T}S\| \leq \|V_{11}^{-T}\| \|S\| = \alpha^{-1} s_n.$$

Therefore, by Theorem 3 and (36) we get the desired inequality. \square

We see that in (37) the ratio of the upper bound and the lower bound is $\frac{1}{\alpha}$. As a consequence, both the bounds estimate $\kappa_g(A, b)$ within $\frac{1}{\alpha}$ times. Therefore, if $\alpha \in (0, 1)$ is near to one, say $\frac{1}{2} < \alpha < 1$, both the bounds are very tight and they estimate $\kappa_g(A, b)$ accurately. We now present a family of examples to illustrate it.

e_p	α	$\hat{\sigma}_n - \sigma_{n+1}$	$\kappa_g(A, b)$	$\alpha^{-1} \frac{\sqrt{\sigma_n^2 + \sigma_{n+1}^2}}{\sigma_n^2 - \sigma_{n+1}^2}$	$\alpha^{-2} \frac{\sqrt{\sigma_n^2 + \sigma_{n+1}^2}}{\sigma_n^2 - \sigma_{n+1}^2}$
10^{-3}	0.516	9.89×10^{-4}	1.38×10^3	1.37×10^3	2.66×10^3
10^{-7}	0.792	9.99×10^{-8}	8.93×10^6	8.93×10^6	1.13×10^7
10^{-10}	0.859	1.00×10^{-10}	8.24×10^9	8.23×10^9	9.59×10^9

Example. We construct TLS problems as in [1, Example 1]: Define

$$[A, b] = Q \begin{bmatrix} \Sigma \\ O \end{bmatrix} V^T \in \mathbb{R}^{m \times (n+1)}, \quad Q = I_m - 2yy^T, \quad V = I_{n+1} - 2zz^T,$$

where $y \in \mathbb{R}^m$ and $z \in \mathbb{R}^{n+1}$ are random unit vectors, and $\Sigma = \text{diag}([n, n-1, \dots, 1, 1 - e_p])$ for a given parameter e_p . Fixing $m = 100$, $n = 20$, and taking $e_p = 10^{-3}, 10^{-7}, 10^{-10}$, respectively, we get three different TLS problems. As indicated by the results of $\kappa_g(A, b)$, as e_p decreases, the TLS problem becomes more ill conditioned. This is also reflected by

the decay of $\hat{\sigma}_n - \sigma_{n+1}$; see [6] and Theorems 8–9. Since α 's are near to one, the lower and upper bounds in (37) estimate the TLS condition numbers accurately.

In view of (37) and the followed comments as well as the above example, it is only possible and significant to improve the bounds essentially for the case that α is small relative to one. Without loss of generality, we assume that

$$0 < \alpha \leq \frac{1}{2}. \quad (39)$$

It will appear that we can establish some lower bound $\underline{\kappa}$ and upper bound $\bar{\kappa}$ such that $\underline{\kappa} < \bar{\kappa} < 4\underline{\kappa}$ holds. As a result, together with (37), we can estimate the TLS condition number $\kappa_g(A, b)$ accurately.

Theorem 6 *Given the TLS problem (1), let $[A, b] = U \text{diag}(\sigma_1, \dots, \sigma_{n+1}) V^T$ be its thin SVD. Denote $[\beta_1, \dots, \beta_n, -\alpha]$ be the last row of V and $S = \text{diag}([s_1, \dots, s_n])$, $s_i = \frac{\sqrt{\sigma_i^2 + \sigma_{n+1}^2}}{\sigma_i^2 - \sigma_{n+1}^2}$, $i = 1, \dots, n$. Then*

$$\begin{aligned} \underline{\kappa} &:= \frac{1}{2} \left(\frac{\alpha^{-2} \sqrt{\beta_1^2 s_1^2 + \dots + \beta_n^2 s_n^2}}{\sqrt{1 - \alpha^2}} + \frac{\sqrt{1 - \alpha^2 - \beta_n^2}}{\sqrt{1 - \alpha^2}} \alpha^{-1} s_n \right) \\ &\leq \kappa_g(A, b) \leq \bar{\kappa} := \frac{\alpha^{-2} \sqrt{\beta_1^2 s_1^2 + \dots + \beta_n^2 s_n^2}}{\sqrt{1 - \alpha^2}} + \alpha^{-1} s_n. \end{aligned}$$

Moreover, if $0 < \alpha \leq \frac{1}{2}$, then

$$\underline{\kappa} < \bar{\kappa} < 4\underline{\kappa}.$$

Proof. Recall that $0 < \alpha < 1$. Noticing that $0 < s_1 \leq s_2 \leq \dots \leq s_n$ and applying Proposition 2, we have

$$\begin{aligned} &\frac{1}{2} \left(\frac{\alpha^{-1} \sqrt{\beta_1^2 s_1^2 + \dots + \beta_n^2 s_n^2}}{\sqrt{1 - \alpha^2}} + \frac{\sqrt{1 - \alpha^2 - \beta_n^2}}{\sqrt{1 - \alpha^2}} s_n \right) \\ &\leq \|V_{11}^{-T} S\| \leq \frac{\alpha^{-1} \sqrt{\beta_1^2 s_1^2 + \dots + \beta_n^2 s_n^2}}{\sqrt{1 - \alpha^2}} + s_n, \end{aligned}$$

where $V_{11} = V(1 : n, 1 : n)$. By Theorem 3, we get the first part of the theorem. Furthermore, we obtain the second part of the theorem by Proposition 3. \square

The significance of this theorem is that we can estimate the condition number $\kappa_g(A, b)$ accurately and cheaply by its lower or upper bound without expensively inverting V_{11}^T in order to compute $\|V_{11}^{-T} S\|$.

5.2 Lower and upper bounds based on a few singular values of A and $[A, b]$

In [15], some bounds for the condition number of the Tikhonov regularization solution have been established using *only* a few singular values of A , where A is the coefficient matrix of the least squares problem under consideration. Such kind of bounds are particularly appealing to the TLS problem since, for a large scale TLS problem, its condition number

formula in Theorem 3 and the bounds in Theorem 6 involve all the singular values of $[A, b]$ and are impractical for computational purpose.

Actually, we have presented such kind of bound (37), but as we commented there, for small α , the bounds may overestimate or underestimate $\kappa_g(A, b)$. In the following, we establish some new lower and upper bounds in the same spirit and finally achieve sharper lower and upper bounds for the case of $0 < \alpha \leq \frac{1}{2}$.

Theorem 7 *For the TLS problem (1), we have*

$$\underline{\kappa}_1 \leq \kappa_g(A, b) \leq \bar{\kappa}_1, \quad (40)$$

where

$$\underline{\kappa}_1 = \frac{\sqrt{1 + \|x_{TLS}\|^2} \sqrt{\hat{\sigma}_{n-1}^2 + \sigma_{n+1}^2}}{\hat{\sigma}_{n-1}^2 - \sigma_{n+1}^2}, \quad \bar{\kappa}_1 = \frac{\sqrt{1 + \|x_{TLS}\|^2} \sqrt{\hat{\sigma}_n^2 + \sigma_{n+1}^2}}{\hat{\sigma}_n^2 - \sigma_{n+1}^2}. \quad (41)$$

Proof. Recall that $r = Ax_{TLS} - b$. Denote

$$M = (A^T A - \sigma_{n+1}^2 I_n)^{-1} ((\|x_{TLS}\|^2 + 1)A^T A + \|r\|^2 I_n) (A^T A - \sigma_{n+1}^2 I_n)^{-1}.$$

From (29), we have

$$KK^T = M - 2\sigma_{n+1}^2 (A^T A - \sigma_{n+1}^2 I_n)^{-1} x_{TLS} x_{TLS}^T (A^T A - \sigma_{n+1}^2 I_n)^{-1}. \quad (42)$$

From now on, denote by $\lambda_i(M)$ the i th algebraically largest eigenvalue of M , where M is an arbitrary symmetric matrix. By the Courant-Fischer theorem [9, p. 182], we get

$$\lambda_2(M) \leq \lambda_1(KK^T). \quad (43)$$

Furthermore, since $2\sigma_{n+1}^2 (A^T A - \sigma_{n+1}^2 I_n)^{-1} x_{TLS} x_{TLS}^T (A^T A - \sigma_{n+1}^2 I_n)^{-1}$ is nonnegative definite, the following inequality holds

$$\lambda_1(KK^T) \leq \lambda_1(M). \quad (44)$$

Combining (43) with (44) and based on (27), we have

$$\sqrt{\lambda_2(M)} \leq \kappa_g(A, b) \leq \sqrt{\lambda_1(M)}.$$

It is easy to verify that the eigenvalues of M form the set

$$\left\{ \frac{(\|x_{TLS}\|^2 + 1)\hat{\sigma}_j^2 + \|r\|^2}{(\hat{\sigma}_j^2 - \sigma_{n+1}^2)^2} \right\}_{j=1}^n.$$

We define the function

$$h(\sigma) = \frac{(\|x_{TLS}\|^2 + 1)\sigma^2 + \|r\|^2}{(\sigma^2 - \sigma_{n+1}^2)^2}, \quad \sigma > \sigma_{n+1}$$

and differentiate it to get

$$h'(\sigma) = \frac{-2\sigma^3(\|x_{TLS}\|^2 + 1) - 2\sigma(\|x_{TLS}\|^2 + 1)\sigma_{n+1}^2 - 4\sigma\|r\|^2}{(\sigma^2 - \sigma_{n+1}^2)^3}.$$

It is seen that $h'(\sigma) < 0$ and $h(\sigma)$ is decreasing in the interval (σ_{n+1}, ∞) . Thus, we get

$$\lambda_1(M) = \frac{(\|x_{TLS}\|^2 + 1)\hat{\sigma}_n^2 + \|r\|^2}{(\hat{\sigma}_n^2 - \sigma_{n+1}^2)^2}, \quad \lambda_2(M) = \frac{(\|x_{TLS}\|^2 + 1)\hat{\sigma}_{n-1}^2 + \|r\|^2}{(\hat{\sigma}_{n-1}^2 - \sigma_{n+1}^2)^2}$$

and

$$\frac{\sqrt{(\|x_{TLS}\|^2 + 1)\hat{\sigma}_{n-1}^2 + \|r\|^2}}{\hat{\sigma}_{n-1}^2 - \sigma_{n+1}^2} \leq \kappa_g(A, b) \leq \frac{\sqrt{(\|x_{TLS}\|^2 + 1)\hat{\sigma}_n^2 + \|r\|^2}}{\hat{\sigma}_n^2 - \sigma_{n+1}^2}.$$

Recalling that $\frac{\|r\|^2}{1 + \|x_{TLS}\|^2} = \sigma_{n+1}^2$, we complete the proof. \square

Remark. In Corollary 1 of [1], the authors prove that

$$\kappa_g(A, b) \leq \frac{\sqrt{1 + \|x_{TLS}\|^2} \sqrt{\sigma_1^2 + \sigma_{n+1}^2}}{\hat{\sigma}_n^2 - \sigma_{n+1}^2}.$$

Since $\hat{\sigma}_n \leq \sigma_n$ and $\sigma_n \leq \sigma_1$, we get

$$\bar{\kappa}_1 \leq \frac{\sqrt{1 + \|x_{TLS}\|^2} \sqrt{\sigma_1^2 + \sigma_{n+1}^2}}{\hat{\sigma}_n^2 - \sigma_{n+1}^2}.$$

Therefore, our $\bar{\kappa}_1$ in (41) is sharper. Moreover, the improvement must be significant when $\frac{\sigma_1}{\hat{\sigma}_n} \gg 1$.

It is seen that the lower and upper bounds in Theorem 7 are marginally different provided that $\hat{\sigma}_n$ and $\hat{\sigma}_{n-1}$ are close. This means that in this case both bounds are very tight. For the case that $\hat{\sigma}_n$ and $\hat{\sigma}_{n-1}$ are not close, we next give a new lower bound that can be better than that in Theorem 7.

Theorem 8 *It holds that*

$$\underline{\kappa}_2 \leq \kappa_g(A, b) \leq \bar{\kappa}_1,$$

where $\bar{\kappa}_1$ is defined as in Theorem 7 and

$$\underline{\kappa}_2 = \frac{\sqrt{1 + \|x_{TLS}\|^2}}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}}.$$

Moreover, when $\hat{\sigma}_{n-1} \geq \sigma_{n+1} + \sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}$, we have

$$\underline{\kappa}_1 \leq \underline{\kappa}_2.$$

Proof. Denote $P = A^T A - \sigma_{n+1}^2 I_n$. From (30), we have

$$\frac{1}{\|x_{TLS}\|^2 + 1} K K^T = P^{-1} + 2\sigma_{n+1}^2 P^{-1} \left(I_n - \frac{x_{TLS} x_{TLS}^T}{1 + \|x_{TLS}\|^2} \right) P^{-1}.$$

Since the second term in the right-hand side of the above relation is positive definite, we have

$$(\|x_{TLS}\|^2 + 1)\lambda_1(P^{-1}) \leq \lambda_1(K K^T),$$

that is,

$$\frac{\|x_{TLS}\|^2 + 1}{\hat{\sigma}_n^2 - \sigma_{n+1}^2} \leq \kappa_g^2(A, b),$$

which used (27). Thus, we obtain the first part of the theorem.

The second part of the theorem is obtained by noting

$$\frac{\sqrt{\hat{\sigma}_{n-1}^2 + \sigma_{n+1}^2}}{\hat{\sigma}_{n-1}^2 - \sigma_{n+1}^2} < \frac{1}{\hat{\sigma}_{n-1} - \sigma_{n+1}} \leq \frac{1}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}}$$

under the assumption that $\hat{\sigma}_{n-1} - \sigma_{n+1} \geq \sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}$. \square

Remark 1. At first glance, the assumption in the second part of the theorem seems not so direct but we can justify that it indeed implies that $\hat{\sigma}_n$ and $\hat{\sigma}_{n-1}$ are not close. Actually, it is direct to verify that the second part of Theorem 8 holds under a slightly stronger but much simpler condition that

$$\hat{\sigma}_{n-1} \geq 2\hat{\sigma}_n.$$

Remark 2. From

$$\frac{\bar{\kappa}_1}{\underline{\kappa}_2} = \frac{\sqrt{\hat{\sigma}_n^2 + \sigma_{n+1}^2}}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}} = \sqrt{\frac{1 + \frac{\sigma_{n+1}^2}{\hat{\sigma}_n^2}}{1 - \frac{\sigma_{n+1}^2}{\hat{\sigma}_n^2}}},$$

it is seen that $\frac{\bar{\kappa}_1}{\underline{\kappa}_2} > 1$ provided $\sigma_{n+1} > 0$. Only for $\sigma_{n+1} = 0$, $\bar{\kappa}_1 = \underline{\kappa}_2$ holds. At this time, $b \in \mathcal{R}(A)$ and $r = 0$.

We observe that the bounds for $\kappa_g(A, b)$ in Theorem 8 are tight when $\frac{\sigma_{n+1}}{\hat{\sigma}_n}$ is considerably smaller than one. On the other hand, if $\frac{\sigma_{n+1}}{\hat{\sigma}_n}$ is not small, these bounds may not be tight. For this case, we will present a new upper bound that may better estimate $\kappa_g(A, b)$.

Keep (36) and (39) in mind. Based on Propositions 2–3, we establish the following theorem.

Theorem 9 *If $0 < \alpha \leq \frac{1}{2}$, then*

$$\underline{\kappa}_2 := \frac{\sqrt{1 + \|x_{TLS}\|^2}}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}} \leq \kappa_g(A, b) < \bar{\kappa}_2 := \sqrt{\frac{1 + 31\rho^2}{1 - \rho^2}} \frac{\sqrt{1 + \|x_{TLS}\|^2}}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}}, \quad (45)$$

where $\rho = \frac{\sigma_{n+1}}{\sigma_n}$.

Proof. The lower bound is the same as that in Theorem 8. We only need to prove the right-hand side of (45). As before, let $[A, b] = U \text{diag}(\sigma_1, \dots, \sigma_{n+1}) V^T$ be its thin SVD with $V_{11} = V(1:n, 1:n)$. From (30), (31) and (33), we get

$$\begin{aligned} \frac{1}{\|x_{TLS}\|^2 + 1} K K^T &= P^{-1} + 2\sigma_{n+1}^2 P^{-1} \left(I_n - \frac{x_{TLS} x_{TLS}^T}{1 + \|x_{TLS}\|^2} \right) P^{-1}, \\ &= V_{11}^{-T} \Lambda^{-1} V_{11}^{-1} + 2\sigma_{n+1}^2 V_{11}^{-T} \Lambda^{-2} V_{11}^{-1} := P^{-1} + C, \end{aligned} \quad (46)$$

where $P = A^T A - \sigma_{n+1}^2 I_n$, $\Lambda = \text{diag}([\sigma_1^2 - \sigma_{n+1}^2, \dots, \sigma_n^2 - \sigma_{n+1}^2])$. Denote

$$\begin{aligned} D &= \text{diag}([d_1, \dots, d_n]), \quad d_i = \frac{\sigma_{n+1}}{\sigma_i^2 - \sigma_{n+1}^2}, \quad i = 1, \dots, n, \\ T &= \text{diag}([t_1, \dots, t_n]), \quad t_i = \frac{1}{\sqrt{\sigma_i^2 - \sigma_{n+1}^2}}, \quad i = 1, \dots, n. \end{aligned}$$

Then $P^{-1} = (V_{11}^{-T} T) (T V_{11}^{-1})$ and $C = 2 (V_{11}^{-T} D) (D V_{11}^{-1})$.

Note that $0 < d_1 \leq d_2 \leq \dots \leq d_n$ and $0 < t_1 \leq t_2 \leq \dots \leq t_n$. From Proposition 2, we get

$$\begin{aligned} & \frac{1}{2} \left(\frac{\alpha^{-1} \sqrt{\beta_1^2 d_1^2 + \dots + \beta_n^2 d_n^2}}{\sqrt{1 - \alpha^2}} + \frac{\sqrt{1 - \alpha^2 - \beta_n^2}}{\sqrt{1 - \alpha^2}} d_n \right) \\ & \leq \|V_{11}^{-T} D\| \leq \frac{\alpha^{-1} \sqrt{\beta_1^2 d_1^2 + \dots + \beta_n^2 d_n^2}}{\sqrt{1 - \alpha^2}} + d_n \end{aligned} \quad (47)$$

and

$$\begin{aligned} & \frac{1}{2} \left(\frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \dots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + \frac{\sqrt{1 - \alpha^2 - \beta_n^2}}{\sqrt{1 - \alpha^2}} t_n \right) \\ & \leq \|V_{11}^{-T} T\| \leq \frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \dots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + t_n, \end{aligned}$$

respectively, where $[\beta_1, \dots, \beta_n, -\alpha]$ is the last row of V as defined previously. Define $k_n = \frac{d_n}{t_n} = \frac{\sigma_{n+1}}{\sqrt{\sigma_n^2 - \sigma_{n+1}^2}}$. Then

$$\frac{d_1}{t_1} = \frac{\sigma_{n+1}}{\sqrt{\sigma_1^2 - \sigma_{n+1}^2}} \leq k_n, \dots, \frac{d_{n-1}}{t_{n-1}} = \frac{\sigma_{n+1}}{\sqrt{\sigma_{n-1}^2 - \sigma_{n+1}^2}} \leq k_n.$$

Thus, from (47) we get

$$\frac{1}{\sqrt{2}} \|C\|^{\frac{1}{2}} = \|V_{11}^{-T} D\| \leq k_n \left(\frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \dots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + t_n \right). \quad (48)$$

For the lower and upper bounds on $\|V_{11}^{-T} T\|$ above, Propositions 2–3 tell us that

$$\begin{aligned} \frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \dots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + t_n &< 2 \left(\frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \dots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + \frac{\sqrt{1 - \alpha^2 - \beta_n^2}}{\sqrt{1 - \alpha^2}} t_n \right) \\ &< 4 \|V_{11}^{-T} T\|. \end{aligned} \quad (49)$$

Therefore, based on (48) and (49), we obtain

$$\frac{1}{\sqrt{2}} \|C\|^{\frac{1}{2}} < 4k_n \|V_{11}^{-T} T\| = 4k_n \|P^{-1}\|^{\frac{1}{2}}$$

and

$$\|C\| < 32k_n^2 \|P^{-1}\|. \quad (50)$$

Combining (46) with (50) and based on (27), we get

$$\begin{aligned}\kappa_g(A, b) = \|K\| = \|KK^T\|^{\frac{1}{2}} &< \sqrt{1 + 32k_n^2} \sqrt{1 + \|x_{TLS}\|^2} \|P^{-1}\|^{\frac{1}{2}} \\ &= \sqrt{\frac{1 + 31\rho^2}{1 - \rho^2}} \frac{\sqrt{1 + \|x_{TLS}\|^2}}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}}.\end{aligned}$$

□

Remark. It is clear that the bounds in Theorem 9 are tight when $\rho = \frac{\sigma_{n+1}}{\sigma_n}$ is considerably smaller than one. Note that the lower and upper bounds in Theorem 8 differ considerably when $\frac{\sigma_{n+1}}{\hat{\sigma}_n}$ is close to one. The result in this theorem is of particular importance when $\frac{\sigma_{n+1}}{\hat{\sigma}_n}$ is close to one, since the upper bound here can be considerably sharper than that in Theorem 8 if only $\rho = \frac{\sigma_{n+1}}{\sigma_n}$ is small.

The improvement of $\bar{\kappa}_2$ over $\bar{\kappa}_1$ can be illustrated as follows. For $\rho = \frac{\sigma_{n+1}}{\sigma_n}$ small, we have

$$\bar{\kappa}_2^{\text{rel}} := \frac{\bar{\kappa}_2}{\|x_{TLS}\|} \| [A, b] \|_F = \sqrt{\frac{1 + 31\rho^2}{1 - \rho^2}} \frac{\sqrt{1 + \|x_{TLS}\|^2}}{\|x_{TLS}\|} \frac{\| [A, b] \|_F}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}},$$

an upper bound for $\kappa_g^{\text{rel}}(A, b)$, is a moderate multiple of $\frac{1}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}}$, while

$$\bar{\kappa}_1^{\text{rel}} := \frac{\bar{\kappa}_1}{\|x_{TLS}\|} \| [A, b] \|_F = \frac{\sqrt{1 + \|x_{TLS}\|^2}}{\|x_{TLS}\|} \frac{\sqrt{\hat{\sigma}_n^2 + \sigma_{n+1}^2}}{\hat{\sigma}_n^2 - \sigma_{n+1}^2} \| [A, b] \|_F$$

is a moderate multiple of $\frac{1}{\hat{\sigma}_n^2 - \sigma_{n+1}^2}$. So the improvement of $\bar{\kappa}_2^{\text{rel}}$ over $\bar{\kappa}_1^{\text{rel}}$ becomes significant as σ_{n+1} and $\hat{\sigma}_n$ are close.

Golub and Van Loan [6] derive an upper bound for the relative condition number for the TLS problem, which, in our notation and case, is simplified as

$$\kappa_{TLS}^{\text{rel}}(A, b) := \frac{9\sigma_1}{\sigma_n - \sigma_{n+1}} \left(1 + \frac{\|b\|}{\hat{\sigma}_n - \sigma_{n+1}} \right) \frac{\| [A, b] \|_F}{\|b\| - \sigma_{n+1}}. \quad (51)$$

We will numerically illustrate improvements of our bounds $\bar{\kappa}_1^{\text{rel}}$ and $\bar{\kappa}_2^{\text{rel}}$ over (51) in the next section.

6 Numerical experiments

We present numerical experiments to illustrate the tightness of the bounds in Theorems 8–9 and to show that our upper bounds can be much better than Golub-Van Loan's upper bound (51) in [6]. For a given TLS problem, the TLS solution is computed by (4). All the experiments were run using Matlab 7.8.0 with the machine precision $\epsilon_{\text{mach}} = 2.22 \times 10^{-16}$ under the Microsoft Windows XP operating system. When α is near to one, it is trivial to estimate the TLS condition number since the lower and upper bounds in (37) are both sharp in this case. Next we will be concerned with only the case that α is not near to one. For all the test problems, we always have $0 < \alpha < \frac{1}{2}$.

Example 1. The data $A \in \mathbb{R}^{m \times (m-2)}$, $b \in \mathbb{R}^m$ are taken from [19]:

$$A = \begin{bmatrix} m-1 & -1 & \cdots & -1 \\ -1 & m-1 & \cdots & -1 \\ \vdots & \vdots & \cdots & \vdots \\ -1 & -1 & \cdots & m-1 \\ -1 & -1 & \cdots & -1 \\ -1 & -1 & \cdots & -1 \end{bmatrix}, \quad b = \begin{bmatrix} -1 \\ -1 \\ \vdots \\ -1 \\ m-1 \\ -1 \end{bmatrix}.$$

So the exact

$$x_{TLS} = [-1, -1, \dots, -1]^T \in \mathbb{R}^{m-2}, \quad \hat{\sigma}_n = \sqrt{2m}, \quad \sigma_{n+1} = \sqrt{m}.$$

m	σ_{n+1}/σ_n	$\sigma_{n+1}/\hat{\sigma}_n$	$\kappa_g^{\text{rel}}(A, b)$	$\underline{\kappa}_2^{\text{rel}}$	$\bar{\kappa}_2^{\text{rel}}$	$\bar{\kappa}_1^{\text{rel}}$	$\kappa_{TLS}^{\text{rel}}(A, b)$
200	7.07×10^{-2}	7.07×10^{-1}	2.01×10^2	2.00×10^2	2.15×10^2	3.46×10^2	5.15×10^3
500	4.47×10^{-2}	7.07×10^{-1}	5.01×10^2	5.00×10^2	5.15×10^2	8.65×10^2	1.21×10^4
1000	3.16×10^{-2}	7.07×10^{-1}	1.00×10^3	1.00×10^3	1.02×10^3	1.73×10^3	2.35×10^4

Table 1: Example 1

In Table 1, we list the results of the relative TLS condition number $\kappa_g^{\text{rel}}(A, b)$ and its bounds

$$\underline{\kappa}_2^{\text{rel}} := \frac{\underline{\kappa}_2}{\|x_{TLS}\|} \|[A, b]\|_F, \quad \bar{\kappa}_2^{\text{rel}} := \frac{\bar{\kappa}_2}{\|x_{TLS}\|} \|[A, b]\|_F, \quad \bar{\kappa}_1^{\text{rel}} := \frac{\bar{\kappa}_1}{\|x_{TLS}\|} \|[A, b]\|_F$$

and $\kappa_{TLS}^{\text{rel}}(A, b)$ (see (51)), where $\underline{\kappa}_2$ and $\bar{\kappa}_2$ are defined in (45), $\bar{\kappa}_1$ is defined in (41).

We can see that the test TLS problems are well conditioned. Both the distance of σ_{n+1} and $\hat{\sigma}_n$ and that of σ_{n+1} and σ_n are not very small so that $\underline{\kappa}_2^{\text{rel}}$, $\bar{\kappa}_2^{\text{rel}}$ and $\bar{\kappa}_1^{\text{rel}}$ all estimate $\kappa_g^{\text{rel}}(A, b)$ accurately. $\kappa_{TLS}^{\text{rel}}(A, b)$ is also good but is not as good as our bounds, and it overestimates $\kappa_g^{\text{rel}}(A, b)$ by one to two orders.

Example 2. In this example, we take the TLS problem from [12]. Specifically, an $m \times (m - 2\omega)$ convolution matrix \bar{T} is constructed to have the first column

$$t_{i,1} = \begin{cases} \frac{1}{\sqrt{2\pi\beta^2} \exp\left[\frac{-(\omega-i+1)^2}{2\beta^2}\right]} & i = 1, 2, \dots, 2\omega + 1, \\ 0 & \text{otherwise,} \end{cases}$$

and the first row

$$t_{1,j} = \begin{cases} t_{1,1} & \text{if } j = 1, \\ 0 & \text{otherwise,} \end{cases}$$

where $\beta = 1.25$ and $\omega = 8$. A Toeplitz matrix A and a right-hand side vector b are constructed as $A = \bar{T} + E$ and $b = \bar{g} + e$, where $\bar{g} = [1, \dots, 1]^T$, E is a random Toeplitz matrix with the same structure as \bar{T} and e is a random vector. The entries in E and e are generated randomly from a normal distribution with mean zero and variance one, and scaled so that

$$\|e\| = \gamma \|\bar{g}\|, \quad \|E\| = \gamma \|\bar{T}\|, \quad \gamma = 0.001.$$

m	σ_{n+1}/σ_n	$\sigma_{n+1}/\hat{\sigma}_n$	$\kappa_g^{\text{rel}}(A, b)$	$\underline{\kappa}_2^{\text{rel}}$	$\bar{\kappa}_2^{\text{rel}}$	$\bar{\kappa}_1^{\text{rel}}$	$\kappa_{TLS}^{\text{rel}}(A, b)$
100	0.964	$1 - 6.08 \times 10^{-8}$	3.41×10^7	3.24×10^7	6.68×10^8	1.31×10^{11}	4.70×10^{17}
300	0.996	$1 - 3.67 \times 10^{-8}$	8.11×10^7	7.21×10^7	4.45×10^9	3.76×10^{11}	2.03×10^{19}
500	0.998	$1 - 6.76 \times 10^{-8}$	8.01×10^7	7.07×10^7	6.36×10^9	2.72×10^{11}	4.13×10^{19}

Table 2: Example 2

In this example, for each test TLS problem, we compute the same quantities as those in Table 1. As indicated by the $\kappa_g^{\text{rel}}(A, b)$'s, these TLS problems are all ill conditioned. Their ill conditioning is also reflected by the fact that σ_{n+1} and $\hat{\sigma}_n$ are close. As estimates of the relative condition number $\kappa_g^{\text{rel}}(A, b)$, both the lower bound $\underline{\kappa}_2^{\text{rel}}$ and the upper bound $\bar{\kappa}_2^{\text{rel}}$ are sharp since σ_{n+1} and σ_n are not so close, but the upper bound $\bar{\kappa}_1^{\text{rel}}$ is not tight any longer and overestimates $\kappa_g^{\text{rel}}(A, b)$ by about four orders. Even though it is not satisfying, $\bar{\kappa}_1^{\text{rel}}$ is still much better than $\kappa_{TLS}^{\text{rel}}(A, b)$, which severely overestimates $\kappa_g^{\text{rel}}(A, b)$ by ten to twelve orders. We also comment that $\bar{\kappa}_2^{\text{rel}}$ improves $\bar{\kappa}_1^{\text{rel}}$ by two orders.

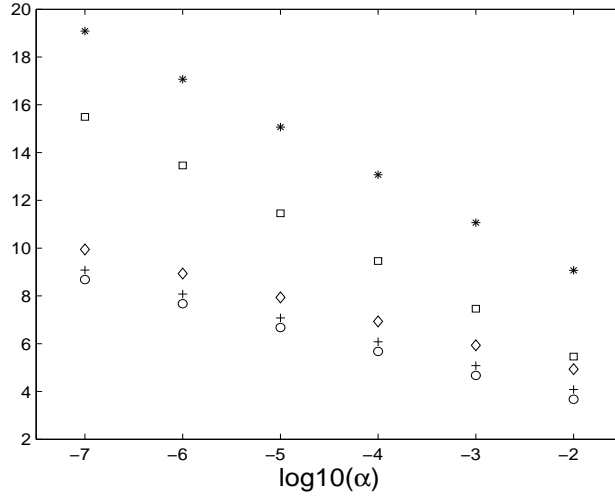


Figure 1: $\log_{10}(\kappa_g^{\text{rel}}(A, b))$ (+), $\log_{10}(\underline{\kappa}_2^{\text{rel}})$ (o), $\log_{10}(\bar{\kappa}_2^{\text{rel}})$ (◇), $\log_{10}(\bar{\kappa}_1^{\text{rel}})$ (□), and $\log_{10}(\kappa_{TLS}^{\text{rel}}(A, b))$ (*) for $(m, n) = (500, 350)$.

Example 3. Keep in mind that the distance between σ_{n+1} and $\hat{\sigma}_n$ can control the conditioning of a TLS problem; see Theorems 8–9 or [6]. In this example, we compare the bounds $\underline{\kappa}_2^{\text{rel}}$, $\bar{\kappa}_2^{\text{rel}}$, $\bar{\kappa}_1^{\text{rel}}$ and $\kappa_{TLS}^{\text{rel}}(A, b)$ for various distances between σ_{n+1} and $\hat{\sigma}_n$. For given m, n , we construct A and b by taking different values of α . Specifically, we generate randomly (with standard normal distribution) two $n \times n$ orthogonal matrices \bar{U} , \bar{V} , and one $m \times (n + 1)$ matrix C_1 , and then compute $C_1 = U \Sigma V_1^T$, the thin SVD of C_1 . Having these fixed matrices \bar{U} , \bar{V} , U and Σ , we take $\alpha = 10^{-2}, 10^{-3}, \dots, 10^{-7}$, run the function

$$C = \text{generator}(n, \alpha, \bar{U}, \bar{V}, U, \Sigma),$$

and set $A = C(:, 1 : n)$, $b = C(:, n + 1)$, respectively. See the pseudo-code function in Appendix for details. In such a way, with $(m, n) = (500, 350)$ and $(1000, 750)$, we generate

100 samples for each α , respectively. For each set of TLS problems with the same α , we compute $\kappa_g^{\text{rel}}(A, b)$, $\underline{\kappa}_2^{\text{rel}}$, $\bar{\kappa}_2^{\text{rel}}$, $\bar{\kappa}_1^{\text{rel}}$ and $\kappa_{TLS}^{\text{rel}}(A, b)$. We plot the (log scale) averages of these quantities and the corresponding (log scale) α in Figures 1–2. We also report the averages of $1 - \frac{\sigma_{n+1}}{\hat{\sigma}_n}$, a measure of the distance between σ_{n+1} and $\hat{\sigma}_n$, in Table 3. We comment that the averages of $\frac{\sigma_{n+1}}{\sigma_n}$ for $(m, n) = (500, 350)$ and $(1000, 750)$ are 0.942 and 0.959, respectively.

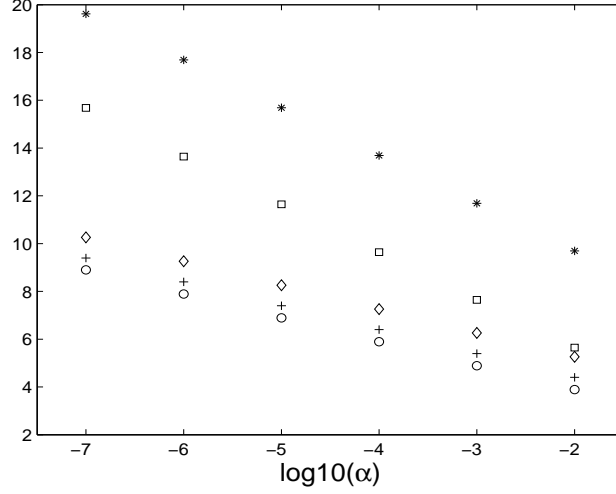


Figure 2: $\log_{10}(\kappa_g^{\text{rel}}(A, b))$ (+), $\log_{10}(\underline{\kappa}_2^{\text{rel}})$ (o), $\log_{10}(\bar{\kappa}_2^{\text{rel}})$ (x), $\log_{10}(\bar{\kappa}_1^{\text{rel}})$ (diamond), and $\log_{10}(\kappa_{TLS}^{\text{rel}}(A, b))$ (*) for $(m, n) = (1000, 750)$.

$(m, n) = (500, 350)$						
α	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
$1 - \frac{\sigma_{n+1}}{\hat{\sigma}_n}$	3.00×10^{-4}	3.01×10^{-6}	3.01×10^{-8}	3.01×10^{-10}	3.01×10^{-12}	2.94×10^{-14}
$(m, n) = (1000, 750)$						
α	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
$1 - \frac{\sigma_{n+1}}{\hat{\sigma}_n}$	3.62×10^{-4}	3.63×10^{-6}	3.63×10^{-8}	3.63×10^{-10}	3.62×10^{-12}	3.54×10^{-14}

Table 3: Example 3

We can see from Figures 1–2 and Table 3 that as α decreases, $\hat{\sigma}_n$ and σ_{n+1} become closer, and the TLS problem becomes more ill conditioned. $\kappa_{TLS}^{\text{rel}}(A, b)$ always severely overestimates $\kappa_g^{\text{rel}}(A, b)$. For $\alpha = 10^{-2}$ in which $\hat{\sigma}_n$ and σ_{n+1} are not very close, $\bar{\kappa}_1^{\text{rel}}$ is tight and estimate $\kappa_g^{\text{rel}}(A, b)$ accurately. For $\alpha = 10^{-3}$, $\hat{\sigma}_n$ and σ_{n+1} are closer. In this case, $\bar{\kappa}_1^{\text{rel}}$ is no longer tight and estimate $\kappa_g^{\text{rel}}(A, b)$ poorly but it still improves $\kappa_{TLS}^{\text{rel}}(A, b)$ by four orders. We observe from Figures 1–2 that $\bar{\kappa}_1^{\text{rel}}$ and $\kappa_{TLS}^{\text{rel}}(A, b)$ estimate $\kappa_g^{\text{rel}}(A, b)$ more poorly as α decreases. Even so, $\bar{\kappa}_1^{\text{rel}}$ is always smaller than $\kappa_{TLS}^{\text{rel}}(A, b)$ by about four orders. In contrast, for all the cases, since σ_n and σ_{n+1} are not so close, $\underline{\kappa}_2^{\text{rel}}$ and $\bar{\kappa}_2^{\text{rel}}$ estimate $\kappa_g^{\text{rel}}(A, b)$ accurately. Particularly, for $\alpha = 10^{-4}$, the upper bound $\bar{\kappa}_2^{\text{rel}}$ improves both $\bar{\kappa}_1^{\text{rel}}$ and $\kappa_{TLS}^{\text{rel}}(A, b)$ very considerably by many orders.

Example 4. In this example, we generate the entries of A and b as random variables normally distributed with mean zero and variance one and observe $\underline{\kappa}_2^{\text{rel}}$, $\bar{\kappa}_2^{\text{rel}}$, $\bar{\kappa}_1^{\text{rel}}$ and

(m, n)	$\kappa_g^{\text{rel}}(A, b)$	$\underline{\kappa}_2^{\text{rel}}$	$\bar{\kappa}_2^{\text{rel}}$	$\bar{\kappa}_1^{\text{rel}}$	$\kappa_{TLS}^{\text{rel}}(A, b)$
(200, 75)	1.33×10^3	4.85×10^2	1.07×10^4	1.35×10^5	8.45×10^8
(500, 350)	1.53×10^4	6.86×10^3	1.09×10^5	2.08×10^7	3.40×10^{10}
(1000, 75)	3.34×10^3	7.28×10^2	2.20×10^4	4.41×10^5	2.34×10^9
(1000, 750)	3.32×10^4	1.26×10^4	2.60×10^5	1.14×10^7	5.47×10^{10}

Table 4: Example 4

$\kappa_{TLS}^{\text{rel}}(A, b)$. For each (m, n) , we conducted 100 random experiments. We report the average results of 100 experiments in Table 4. We observe that, as estimates of $\kappa_g^{\text{rel}}(A, b)$, both $\underline{\kappa}_2^{\text{rel}}$ and $\bar{\kappa}_2^{\text{rel}}$ are tight. The upper bound $\bar{\kappa}_2^{\text{rel}}$ improves $\bar{\kappa}_1^{\text{rel}}$ by one or two orders and improves $\kappa_{TLS}^{\text{rel}}(A, b)$ by about five orders. Clearly, the test TLS problems are quite well conditioned, but $\kappa_{TLS}^{\text{rel}}(A, b)$ is a rather poor upper bound and overestimate $\kappa_g^{\text{rel}}(A, b)$ too much.

7 Concluding Remarks

In the paper, we have studied the SVD-based condition number theory of the TLS problem. For the TLS condition number, we have established a new closed formula. Starting with it, we have derived sharp lower and upper bounds. Importantly and more practically, we have presented both lower and upper bounds that use only the smallest two singular values of A and of $[A, b]$. We have demonstrated the tightness of our bounds by numerical experiments. Throughout the paper, the considered TLS problem is assumed to satisfy condition (2) and has a unique TLS solution. It is significant and important to extend the results presented in the paper to a general generic TLS problem [19, 20] that has non-unique TLS solutions or to the non-generic TLS problem [19]. We will consider these problems in forthcoming papers. Besides, it might be worthwhile to investigate how to apply the core problem theory [17] to study the TLS condition number.

A A pseudo-code of generating test TLS problems

For the TLS problem (1), Lemma 4.3 in [6] gives

$$\frac{|\hat{u}_n^T b|}{2(\hat{\sigma}_n - \sigma_{n+1})} \leq \|x_{TLS}\| \leq \frac{\|b\|}{\hat{\sigma}_n - \sigma_{n+1}}.$$

Equivalently, it holds that

$$\frac{|\hat{u}_n^T b|}{2\|x_{TLS}\|} \leq \hat{\sigma}_n - \sigma_{n+1} \leq \frac{\|b\|}{\|x_{TLS}\|}. \quad (52)$$

Denote $V(n+1, n+1) = -\alpha$ and recall that $\alpha = \frac{1}{\sqrt{1+\|x_{TLS}\|^2}}$. From (52) we see that a small α implies that $\hat{\sigma}_n$ and σ_{n+1} are close in some sense.

The following pseudo-code generates $C = [A, b]$, where $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^n$, it has the thin SVD $C = [A, b] = U\Sigma V^T$ that satisfies $V(n+1, n+1) = -\alpha$, where α is a given parameter such that $0 < \alpha < 1$. The idea of construction comes from Proposition 1.

```

 $C = \text{generator}(n, \alpha, \bar{U}, \bar{V}, U, \Sigma)$ 
%  $n$  : a given positive integer
%  $\alpha$  : a given positive number with  $0 < \alpha < 1$ 
%  $\bar{U}, \bar{V}$  : two  $n \times n$  orthogonal matrices
%  $U$  : an  $m \times (n + 1)$  column orthonormal matrix
%  $\Sigma$  : an  $(n + 1) \times (n + 1)$  diagonal matrix with positive diagonal elements
% Output :  $C = [A, b]$ , where  $A = C(:, 1 : n), b = C(:, n + 1)$ .
 $u = \bar{U}(:, n);$ 
 $vt = \bar{V}(:, n)';$ 
 $V_{11} = \bar{U}(:, 1 : n - 1) * \bar{V}(:, 1 : n - 1)' + \alpha * u * vt;$ 
 $t = \text{sqrt}(1 - \alpha * \alpha);$ 
 $V = [ [V_{11}, t * u]; [t * vt, -\alpha] ];$ 
 $C = U * \Sigma * V';$ 

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